3D Modeling of Metallic Grain Growth

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Abstract

This paper will describe simulating metallic grain growth using our Gradient Weighted Moving Finite Elements code, GRAIN3D. We also describe the set of mesh topology change operations developed to respond to changes in the physical topology such as the collapse of grains and to maintain uniform calculational mesh quality. Validation of the method is demonstrated by comparison to analytic calculations. We present results of multigrain simulations where grain boundaries evolve by mean curvature motion and include results which incorporate grain boundary orientation dependence.

Introduction

Metals important to semiconductor manufacture such as aluminum and copper possess a microstructure consisting of individual grains. The atoms in the grains exist in a crystal lattice, and the lattice orientations of adjacent grains differ. The boundary surfaces between grains are areas of lattice misalignment. In the simplest approximation, this excess energy at the boundaries can be represented as a constant energy density per unit area. As the metal is heated, the grain boundaries move to minimize surface energy in such a way that the normal velocity of a point on the grain boundary is proportional to the mean curvature at that point [1]. While the mean curvature model works well for certain classes of materials, it cannot reproduce the faceting that has been observed in some metals. To model the orientation-dependent grain boundary energy density, we assign orientations to the individual grains and modify the equations of boundary motion accordingly.

Summary of Method

We use Gradient-Weighted Moving Finite Elements [2],[3],[4] to move the network of triangles that corresponds to the grain interfaces. In the mean curvature model of grain growth, the interface surfaces motion is described by

$$v_n = \mu K,$$

where v_n is the normal velocity of the interface, K is the curvature and μ is the mobility which for the simulations presented here is assumed to be constant. Following the derivation given in [5], we obtain a system of 3N ODE's of the form:

$$\mathbf{C(x)}\,\dot{\mathbf{x}} = \mathbf{g(x)}$$

Where N is the number of interface nodes, **x** is the 3N vector containing the coordinates of the interface nodes, **C(x)** is a block structured matrix of inner products of basis functions, and **g(x)** are inner products involving surface curvature. Since K on a piecewise linear manifold is actually a distribution that is zero in the interior of a triangle and infinite on the edges, we smooth the manifold in a small neighborhood of the edges.

Since interface physics supplies only interface velocities, we extend **C** and **g** to allow for moving the tetrahedra attached to the interfaces. Additionally, we add grid viscosity forces to the left hand side to maintain reasonable timestep in the presence of areas of near coplanarity of neighboring interface nodes, and we add quality forces to the right hand side to prevent the collapse of interface triangles and the inversion of volume tetrahedra. The grid forces on the tetrahedra move the grid by acting to minimize the nonuniformities in grid velocity and to improve the grid element quality. These forces will have the effect of overriding physically justified node motion if such motion will cause a tetrahedra to invert. This effect is acceptable with regard to accuracy since it removes only a small fraction of numerical degrees of freedom from the simulation. Application of the grid operations merge, face swap, and edge swap remove such problematic tetrahedra and are discussed in the next section.

Grid Maintenance Operations

A large set of mesh optimization and maintenance operations is required to allow our simulation to survive all the transitions of interface geometry and topology that occur during grain evolution. A first category of mesh operations maintains good element quality and requires a combination of node merging, node smoothing, edge refinement, and face swapping to keep the simulation from prematurely terminating. Interestingly, we have also found that it is impossible to completely de-couple the physical motion of the interface triangles from the conforming tetrahedral mesh that contains them, because of the inevitable presence of "all-surface" tetrahedra (i.e. tetrahedra all of whose vertices lie on the same grain boundaries). These tetrahedra are very flat and have near zero volume and hence are prone to invert as the interface deforms. To prevent element inversion, we have found it is necessary to add artificial forces to the physically justified forces on the interfaces. These artificial forces

keep the simulation "alive" until periodically the worst offending "all-surface" tetrahedra are removed by merging their vertices.

A second category of mesh operations captures changes in interface topology. We have found that it is necessary to keep track of the various connected topological components and determine whether they are on the verge of disappearing or changing as the simulation evolves. For example, for all pairs of grains that touch each other, we monitor the topological component consisting of connected interface triangles between the two grains. If the total surface area of one such component is about to go to zero, a physical topological change is imminent; GRAIN3D detects this change and responds by performing topological operations on the computational tetrahedral mesh. Similar strategies are required to detect other forms of topological change.

In order to monitor the rate of collapse of the assembled connected sets of elements, surface triangles, and interface edges, we maintain a nodal velocity history. The combination of historical rate of collapse and volume collapse indicates that action must be taken to respond to the imminent topological change. We identify the neighborhood surrounding the collapsing feature and refine this neighborhood to provide an epsilon thick buffer region. The encroaching materials are examined to identify a 'winner', and the collapsing feature and its associated epsilon neighborhood are assigned the winner's material. Soon after the material reassignment, the forces on the material interfaces will effectively straighten the interfaces.

Periodically during the grain evolution, the Los Alamos Grid Toolbox, LaGriT [6], is invoked to improve mesh quality. LaGriT provides a mesh optimization operation, "massage", that combines the "merge", "refine" and "recon" basic operations. Massage accepts a refinement length which causes edges longer than the specified length to be bisected, a merge length which causes edges shorter than the specified length to be merged away and a damage tolerance with forbids any operations that would change the shape of material interface by more than the specified damage. All operations are performed in a way that guarantees that the mesh connectivity will not become corrupted and that ensures the integrity of grain interfaces.

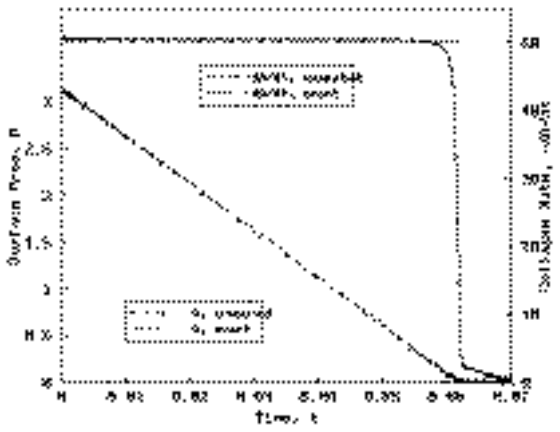
Spherically Symmetric Collapse

The collapse of a spherical grain is solvable analytically assuming that the normal collapse velocity is equal to the curvature. The rate of change of surface area is:

$$dr/dt = K = -2/r$$

$$dA/dt = d(4\pi r^2)/dt = -16\pi$$

We ran the simulation on 42-node, 162-node and 642-node representations of a sphere. In each case the nodes were initially equally spaced at a radius of 0.5. This spacing creates a polygonal representation of the sphere that will have a smaller surface area than a true sphere with the same radius. Figure 1 shows the close agreement of calculation to simulation for the 642-node sphere. Near the terminal time (0.0625) the tetrahedra inside the sphere have collapsed to such a small size that the



tetrahedral quality force dominates and effectively stops the collapse.

Figure 1. *Results for 642 –node sphere run.*

Mean Curvature Example

In this section we show how GRAIN3D evolves a 3D microstructure, successfully maintaining mesh quality and performing necessary topological changes during the course of the calculation. The initial microstructure was obtained via Monte Carlo evolution of a discrete effective spin (Potts) model on the elements of the unstructured tetrahedral grid generated by LaGriT. The Potts model is know to be the discrete analog of curvature driven motion. The initial configuration consisted of 140 grains arrayed in a flat plate. Figure 3, 4 and 5 show three snapshots in the time sequence in which grains shrink and disappear. Note that the grid is maintained throughout the simulation, keeping the number and spacing of the nodes approximately constant. Although only the surface grid is displayed, the quality of the mesh is maintained in the volume as well.

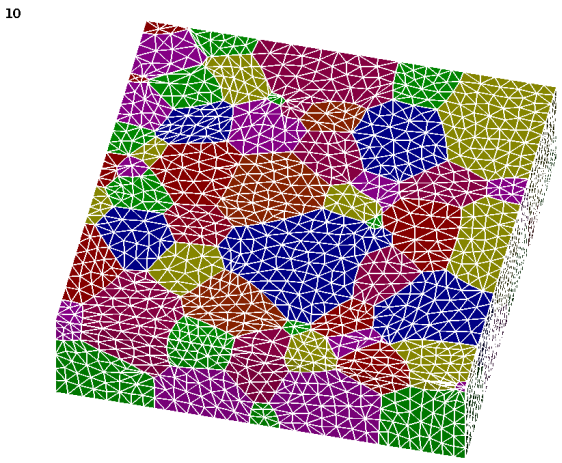


Figure 2. Early timestep in the 140 grain simulation

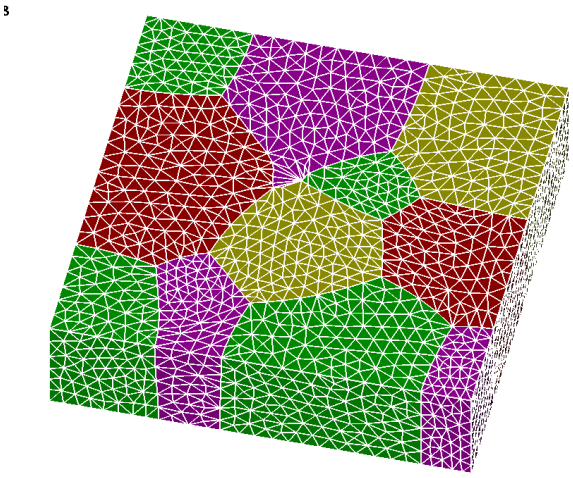


Figure 3. 140 grain growth simulation at t=78.

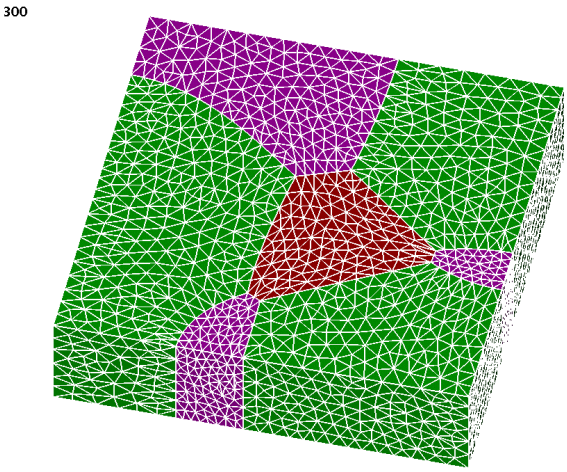


Figure 4. 140 grain growth simulation at t=300.

Grain Boundary Orientation Example

In order to model the faceting behavior found in grain growth in metals such as copper, we have modified the grain growth model to incorporate orientation-dependent grain boundary energy. We use the standard coincident site lattice (CSL) notation to relate the twist, tilt and symmetry parameters to the grain boundary energy. We have fit the parameters to the microscopic calculations for fcc symmetric copper found in Reference [7]. Again the initial microstructure was derived via Monte Carlo evolution of a discrete effective classical spin (Potts) model. The discrete code was modified to allow the Potts spins to live on the nodes rather than on the elements. The initial random node spins were annealed until only five grains remained. Then each grain was assigned an orientation. To remove any artifacts that may have arisen as a result of the discrete methods a few timesteps of mean curvature moving finite elements were executed to reach the microstructure shown in figure 5. We now ran both the mean curvature model and the orientation-dependent model. The results are displayed in figures 6 and 7. Note that the general motion of the interfaces is similar, but that the orientation-dependent model shows steps and facets and grain boundary angles that are forbidden by the mean curvature model.

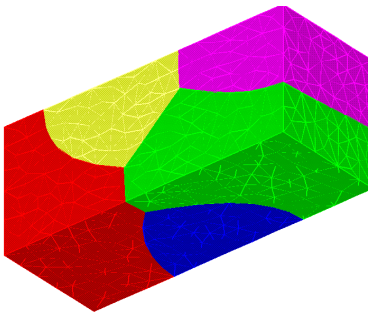


Figure 5. Initial microstructure of a copper line.

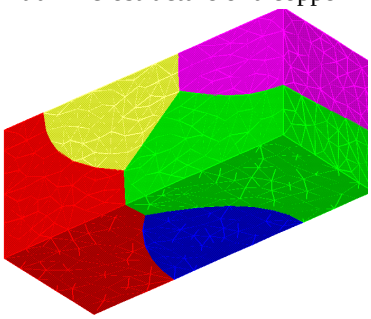


Figure 6. Microstructure of a copper line at t=4, grain interfaces moved using mean curvature.

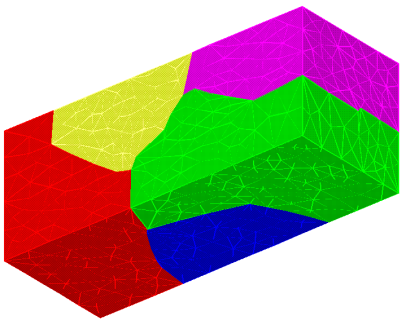


Figure 7. Microstructure of a copper line at t=4, grain interfaces moved using an orientation-dependent model.

Future Plans

Although 3D grain growth data are not readily available, we plan on validating our model against existing 2D data. We also are writing GRAIN2D based also on Gradient-Weighted Moving Finite Elements. We will compare GRAIN2D results against data and against existing codes. At the same time we are incorporating more features into GRAIN3D including modeling thermal effects and the effects of stress.

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